

CHEMISTRY

A EUROPEAN JOURNAL

Supporting Information

© Copyright Wiley-VCH Verlag GmbH & Co. KGaA, 69451 Weinheim, 2008

Functionally Rigid and Degenerate Molecular Shuttles

Il Yoon,^[b] Diego Benítez,^[b] Yan-Li Zhao,^[b] Ognjen Š. Miljanić,^[b] Soo-Young Kim,^[b]

Ekaterina Tkatchouk,^[c] Ken C.-F. Leung,^[b] Saeed I. Khan,^[b]

William A. Goddard III,^[c] and J. Fraser Stoddart*^[a,b]

[a] Department of Chemistry, Northwestern University

2145 Sheridan Road, Evanston, Illinois 60208 (USA)

[b] Department of Chemistry and Biochemistry, University of California, Los Angeles

405 Hilgard Avenue, Los Angeles, California 90095 (USA)

[c] Materials and Process Simulation Center, California Institute of Technology

Pasadena, California 91125 (USA)

Compound Characterization. Figures S1 and S2 portray the ESI-MS spectra of the [2]rotaxane **1**·4PF₆. Figures S3-S6 show 2D COSY NMR spectra of the [2]rotaxane **1**·4PF₆. Figures S7-S9 show 2D COSY NMR spectra of the [2]rotaxane **2**·4PF₆. Figure S10 portrays the VT NMR spectra of the [2]rotaxane **1**·4PF₆. Figures S11-S13 show the cell unit and packing superstructures for the rigid dumbbell **3**.

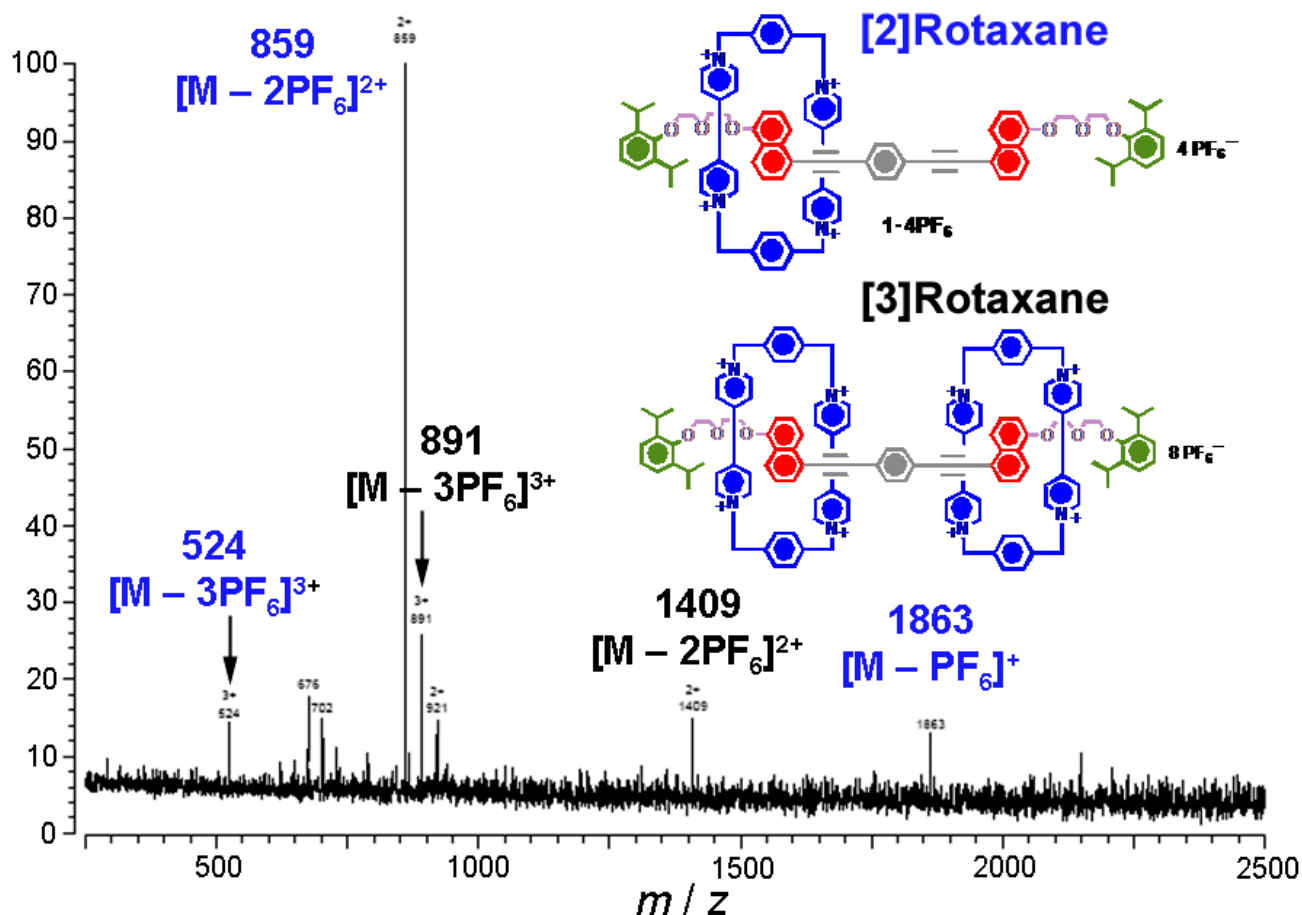


Figure S1. ESI-MS of a mixture of the [2]rotaxane **1**·4PF₆ and the [3]rotaxane

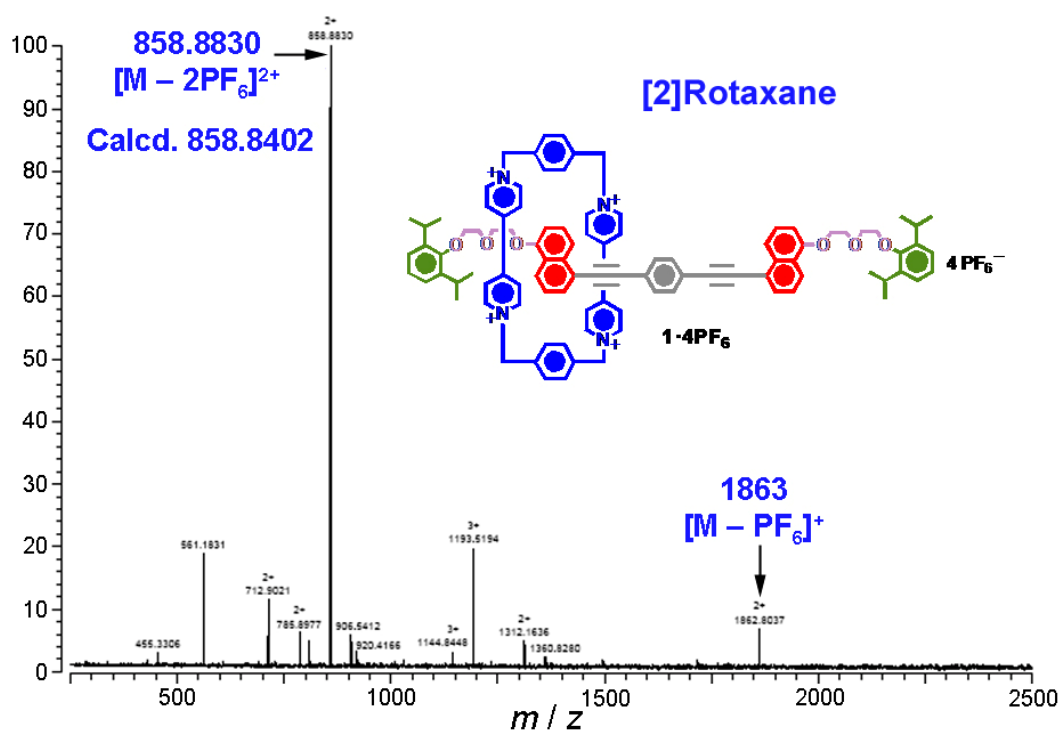


Figure S2. ESI-MS of the [2]rotaxane **1**·4PF₆

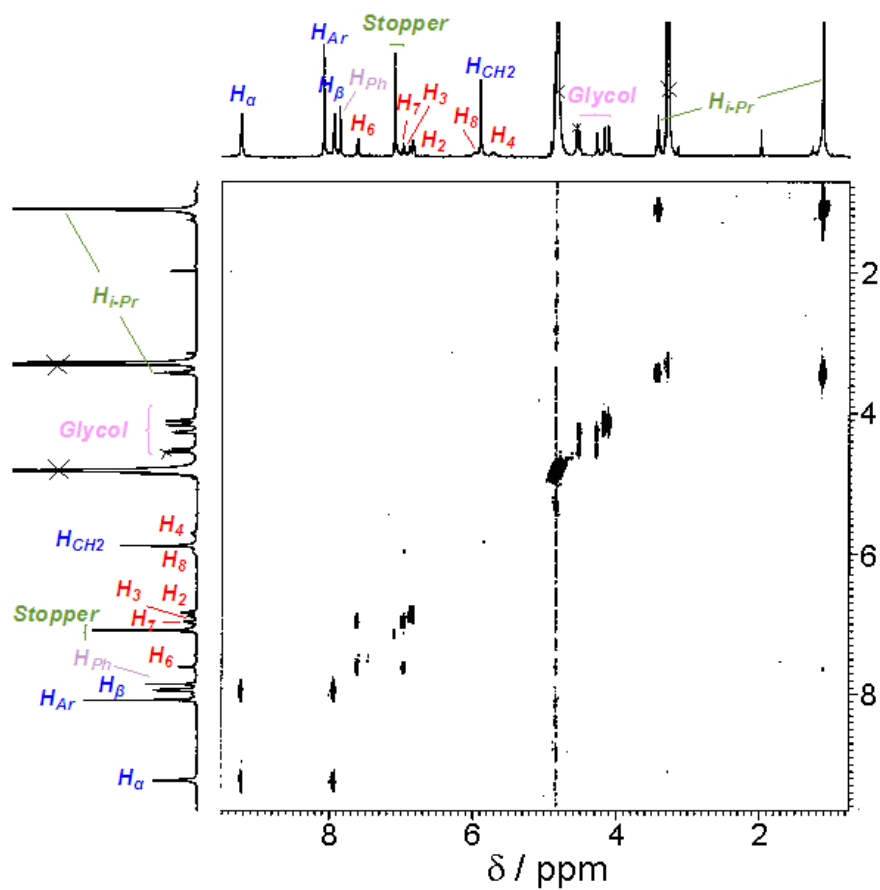


Figure S3. COSY-2D ¹H NMR spectrum of **1**·4PF₆ in CD₃OD at 298 K

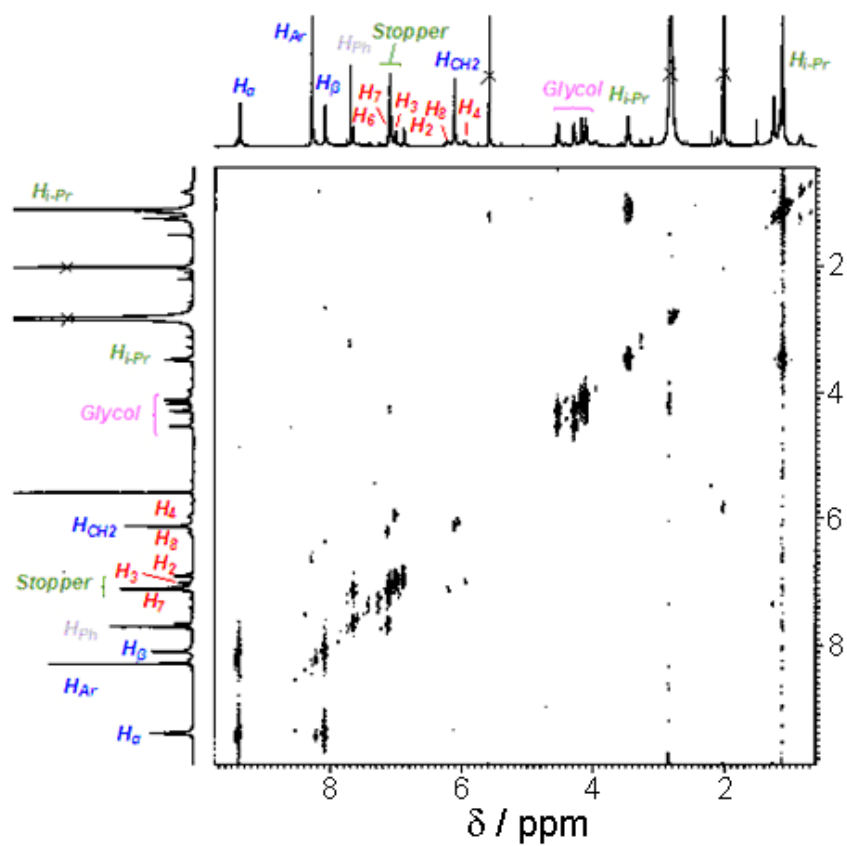


Figure S4. COSY-2D ^1H NMR spectrum of **1**·4PF₆ (500 MHz, CD₃COCD₃, 298 K)

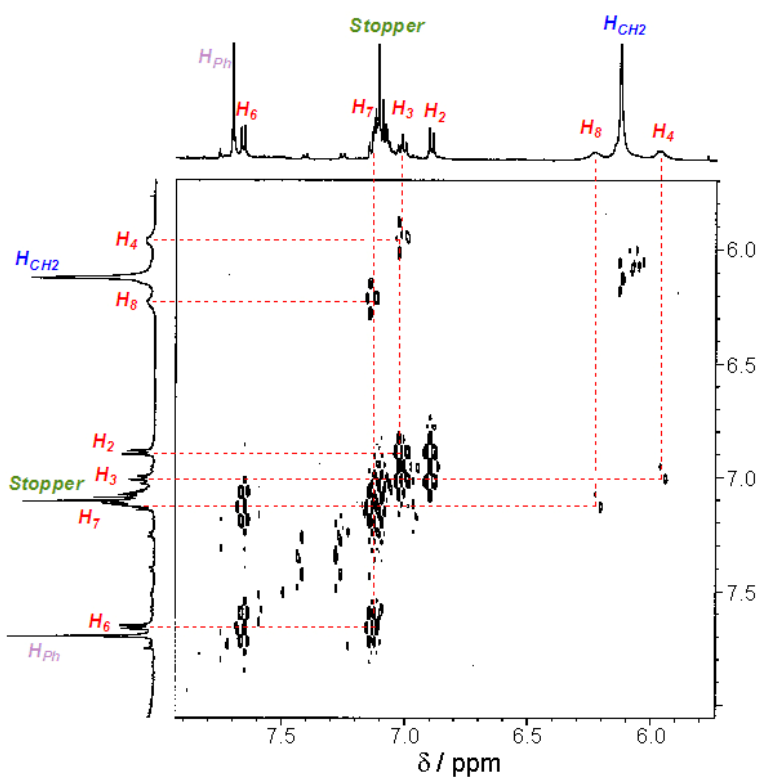


Figure S5. Part of COSY-2D ^1H NMR spectrum of **1**·4PF₆ in CD₃COCD₃ at 298 K

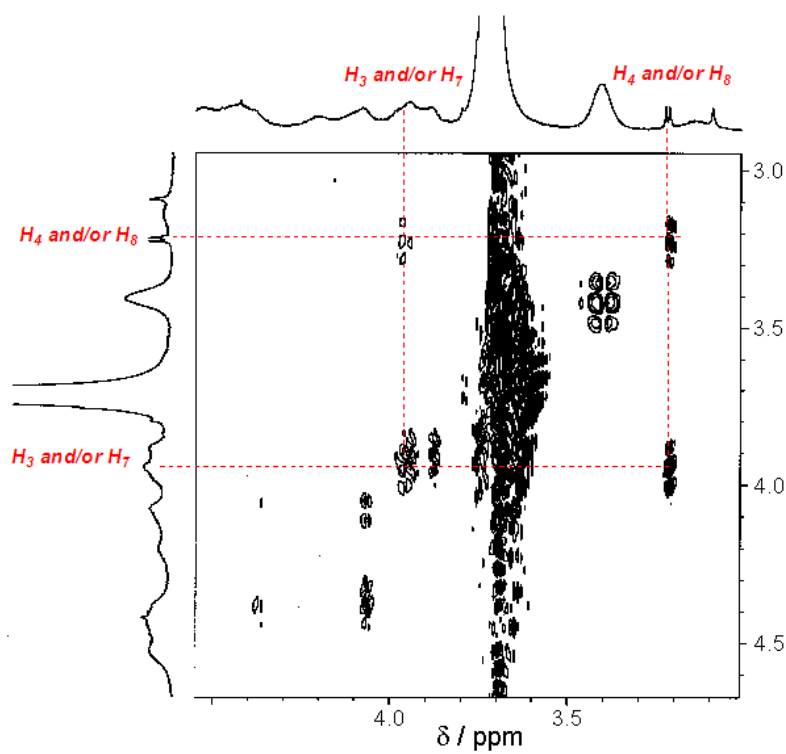


Figure S6. Part of COSY-2D ^1H NMR spectrum of **1**·4PF₆ in CD₃COCD₃ at 190 K

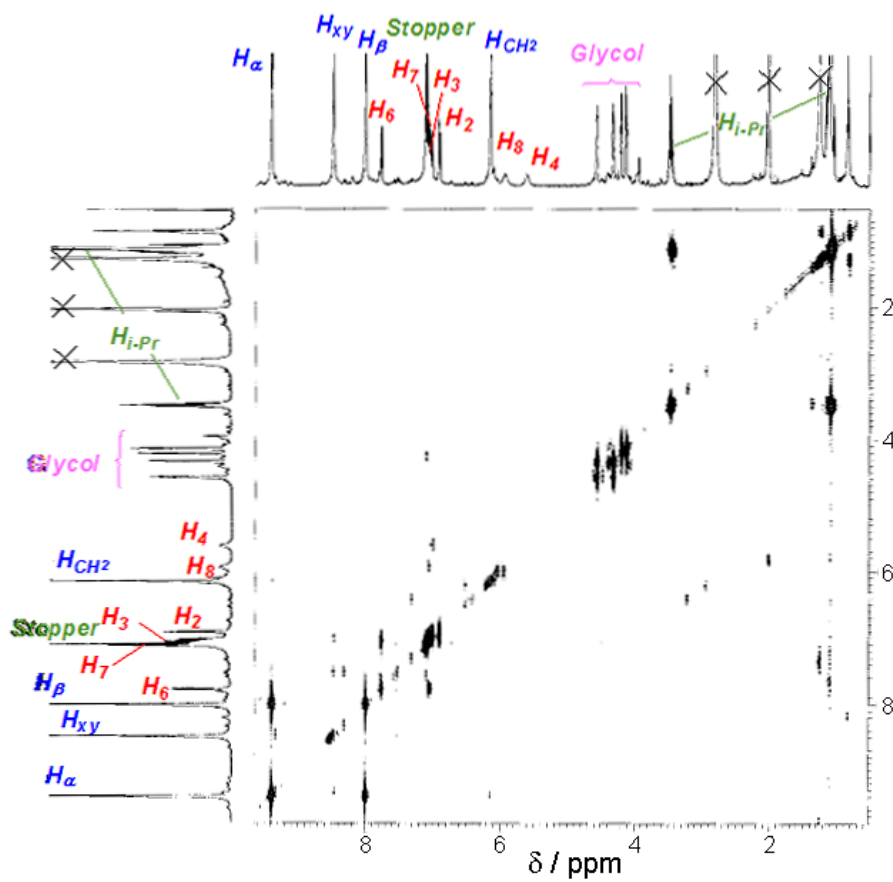


Figure S7. COSY-2D ^1H NMR spectrum of **2**·4PF₆ in CD₃COCD₃ at 298 K

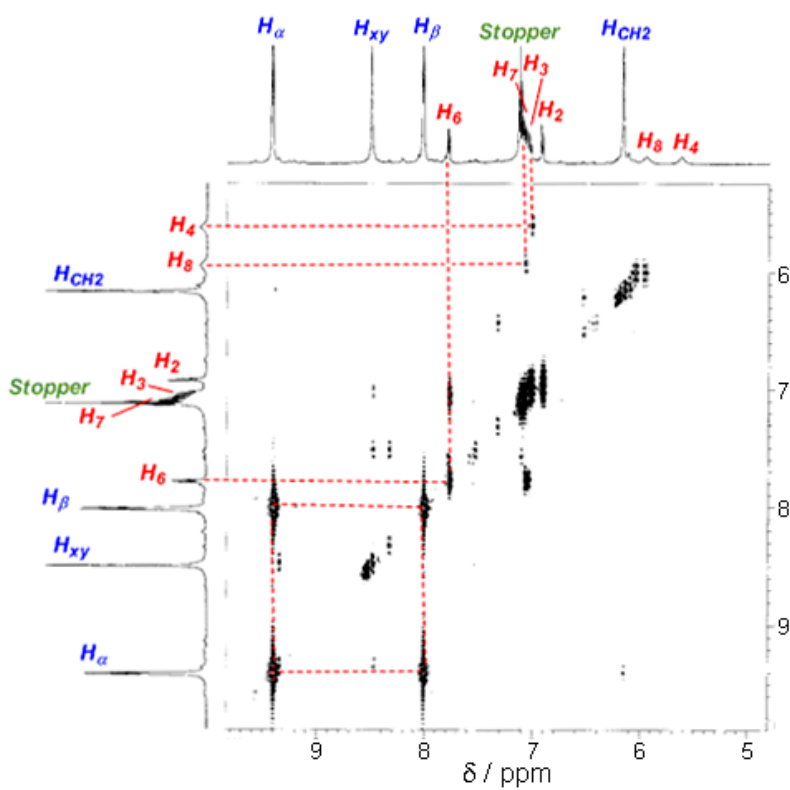


Figure S8. Part of COSY-2D ^1H NMR spectrum of $2\cdot 4\text{PF}_6$ in CD_3COCD_3 at 298 K

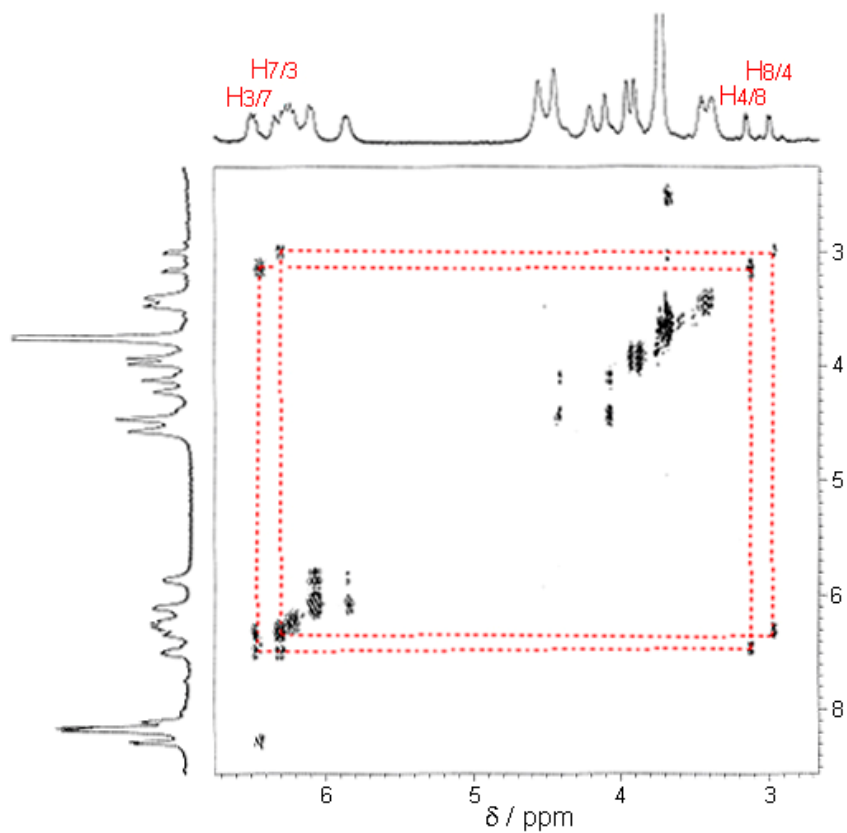


Figure S9. Part of COSY-2D ^1H NMR spectrum of $2\cdot 4\text{PF}_6$ in CD_3COCD_3 at 184 K

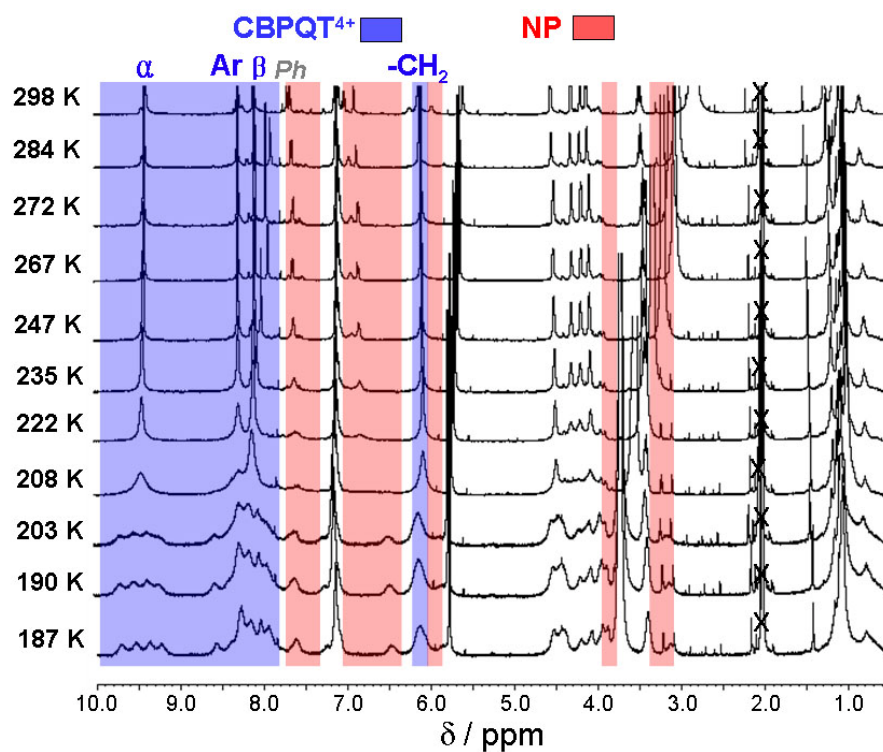


Figure S10. VT-NMR Spectra of **1**·4PF₆ in CD₃COCD₃

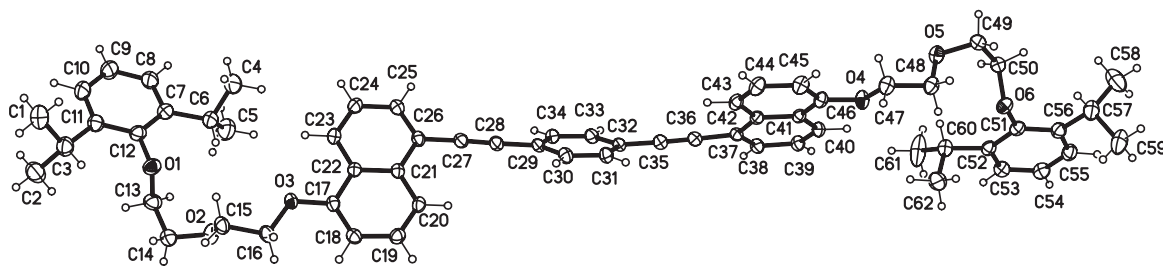


Figure S11. Solid-state structure of rigid dumbbell **3**

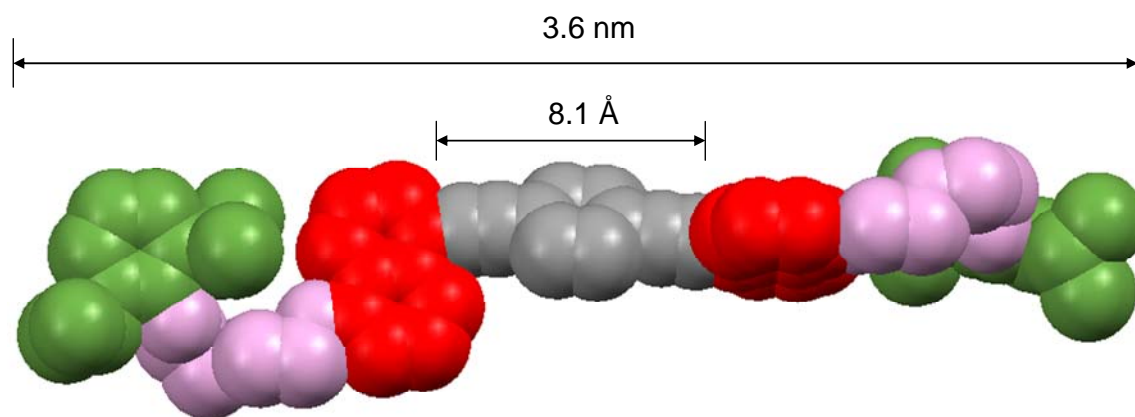


Figure S12. Space-filling representation of **3**. The length of the molecule is 3.6 nm. The length of the ethynyl-phenylene-ethynyl unit as a spacer between two naphthalene units is 8.1 Å

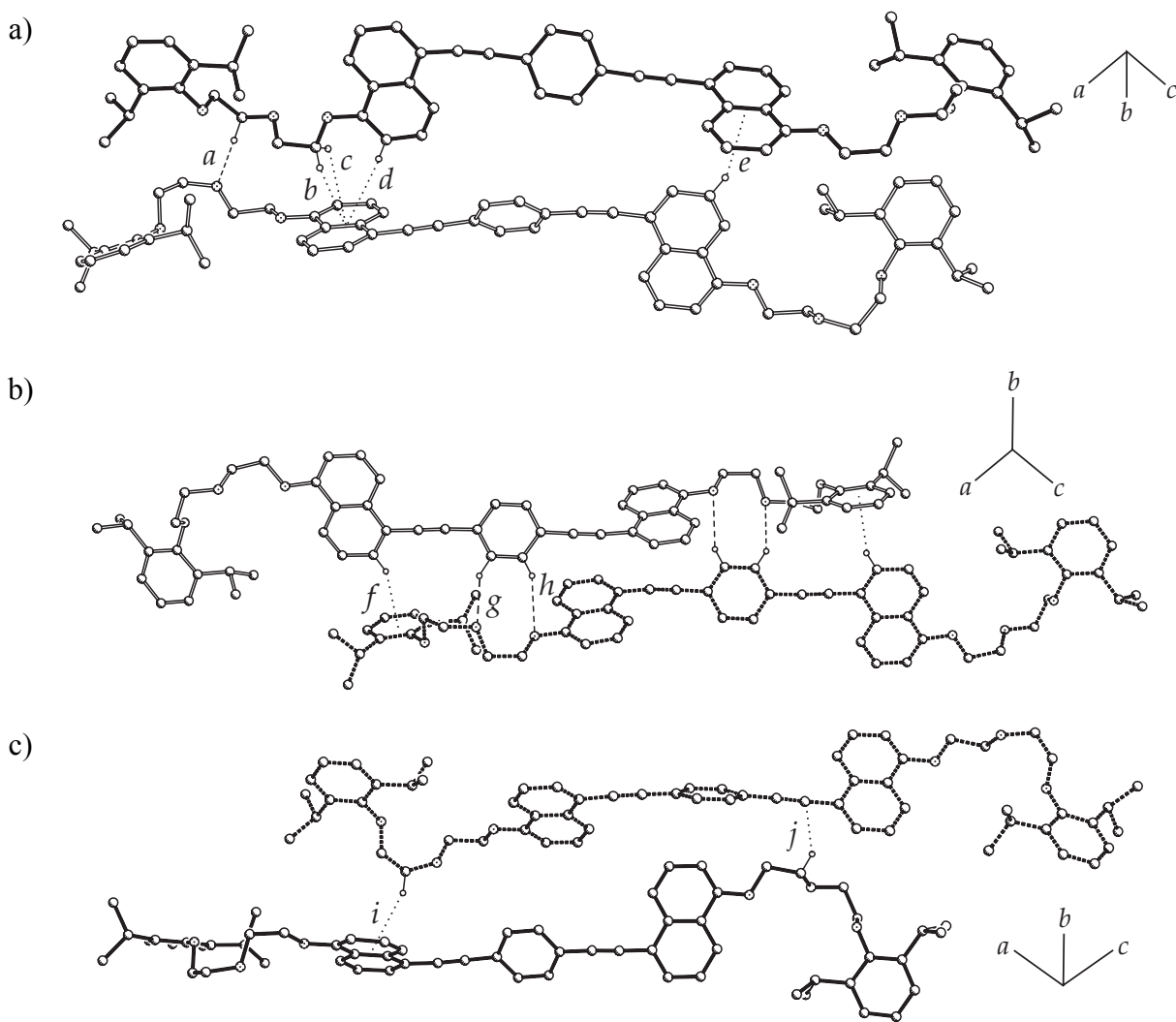


Figure S13. Packing diagram showing the intermolecular [C-H...O] and [C-H...π] interactions in **3**; each molecule has been shown with the same bond type (solid, open, and dashed solid lines, respectively). [C-H...O] interaction geometries {[X...O], [H...O] distances (Å), and [X-H...O] angles (°)}: a) 3.30, 2.46, 146; g) 3.49, 2.69, 142; h) 3.38, 2.53, 147. The [H...π] distances (Å) and [C-H...π] angles (°) for the [C-H...π] interactions are b) 2.86, 118; c) 3.10, 101; d) 3.14, 163; e) 2.89, 159; f) 2.62, 156; i) 3.00, 158; j) 2.87, 134. All hydrogen atoms, except for those involved in [C-H...O] and [C-H...π] interactions, have been omitted for clarity